Understanding Compositional and Morphological Evolution of Graphene-Oxide Quantum Dots Through the Laser Synthesis Process

Damiano Ricciarelli
Simona Filice, Viviana Scuderi, Gaetano Calogero, Ioannis Deretzis, Giuseppe Fisicaro, Silvia Scalese, Antonino La Magna
National Research Council of Italy, Institute for Microelectronics and Microsystems, VIII Strada 5, Catania, Italy
damiano.ricciarelli@cnr.it

Originating from oxidized graphene, graphene oxide (GO) is notably distinguished by its exceptional dispersibility in water and interesting opto-electronical properties. These qualities uniquely qualify GO as a targeted material for both environmental and biomedical applications, where its use in the form of quantum dots notably enhances electro-optical attributes and the material's ability to interface with biological substrates. [1][2] In our study, we irradiated micrometre-sized graphene oxide dispersions in water with a 532 nm laser, aiming for two primary outcomes: (i) reducing GO to recover some of the original electrical and optical properties of graphene, and (ii) creating quantum dots. [3][4] To understand the process of converting GO into quantum dots via laser synthesis, we engaged in density functional theory (DFT) simulations. These simulations focused on examining changes in morphology and oxygen composition evolution of the substrates modelled as nanoribbons (Figure 1a). In particular, we investigated modifications in the UV-VIS spectra and electronic structures through computational methods after sample reduction (Figure 1b), we assessed the impact of 1D and 0D confinement using refined models, and we ultimately compared our theoretical insights with experimental spectra obtained for different laser fluences, clarifying the experimental observations in terms of the aforementioned compositional and morphological alterations.

References

[1] Dikin *et al*, Nature, 448 (2007) 457-460
[2] Pan *et al.*, Advanced Materials, 22 (2010) 734-738
[3] Buccheri *et al.*, Nanotechnology, 24 (2016) 245704
[4] Filice *et al.*, Materials Science in Semiconductor Processing, 42 (2016) 50-53

Figures

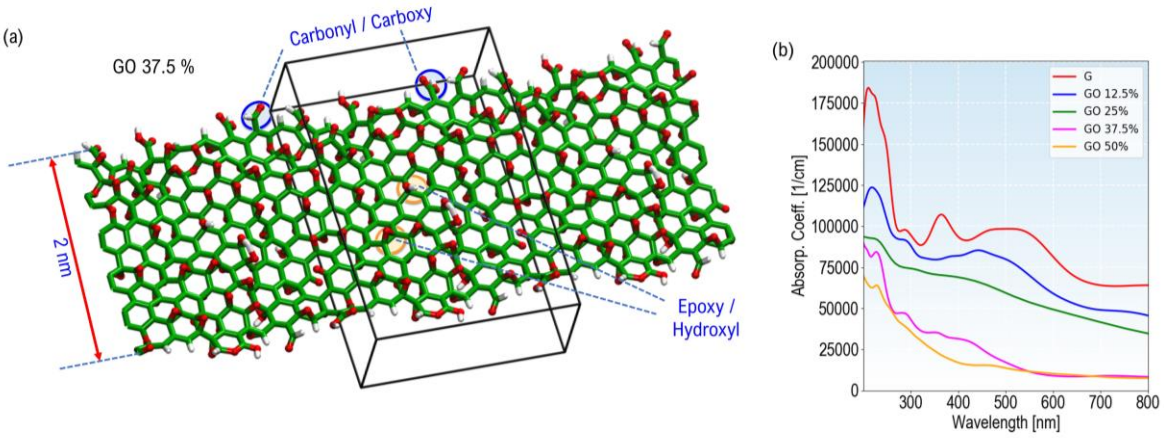

Figure 1: (a) Nanoribbon used to model GO at a % oxygen of 37.5 %, (b) variations on the calculated UV-VIS spectra obtained by varying oxygen composition.